Supporting Information

Title: Repurposing of FDA-Approved Toremifene to Treat COVID-19 by blocking the spike glycoprotein and NSP14 of SARS-CoV-2

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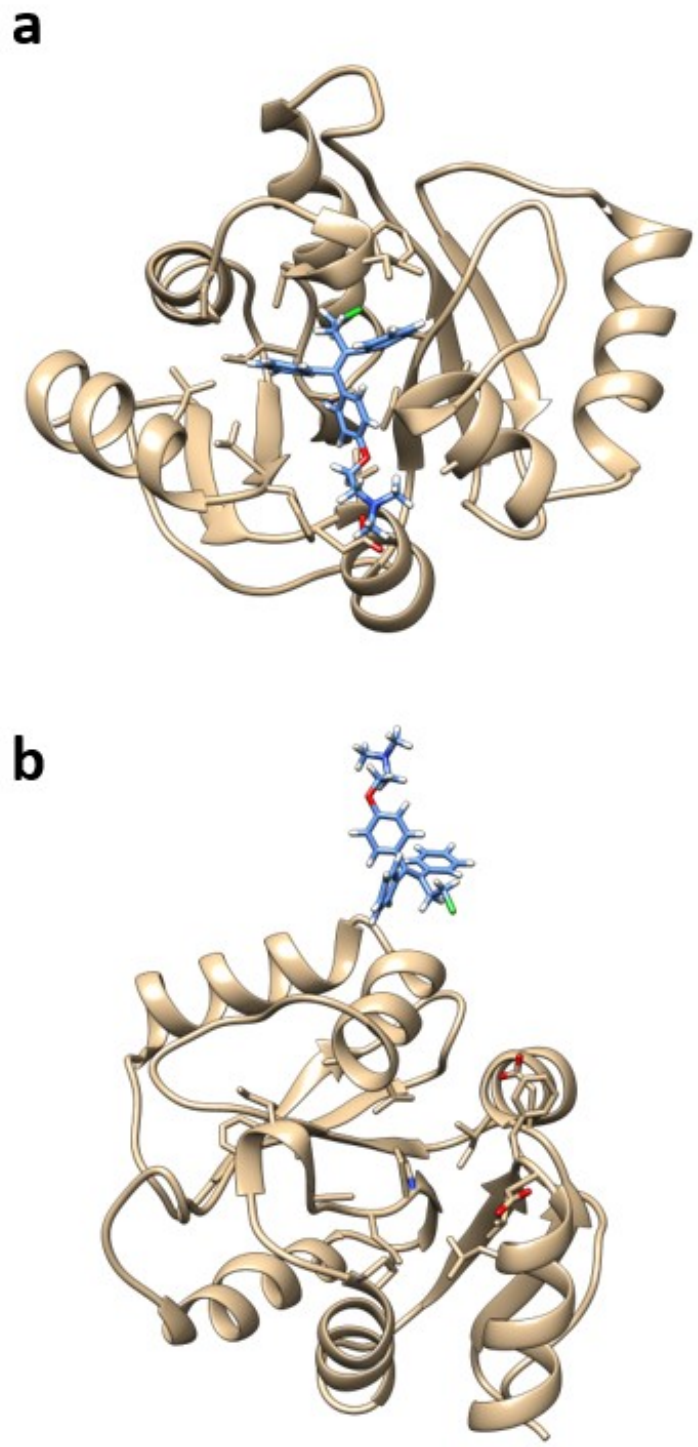

Figure S1: NSP3 (PL-PRO) in the initial docked conformation (a) and at 34.4 nanoseconds of simulation (b).

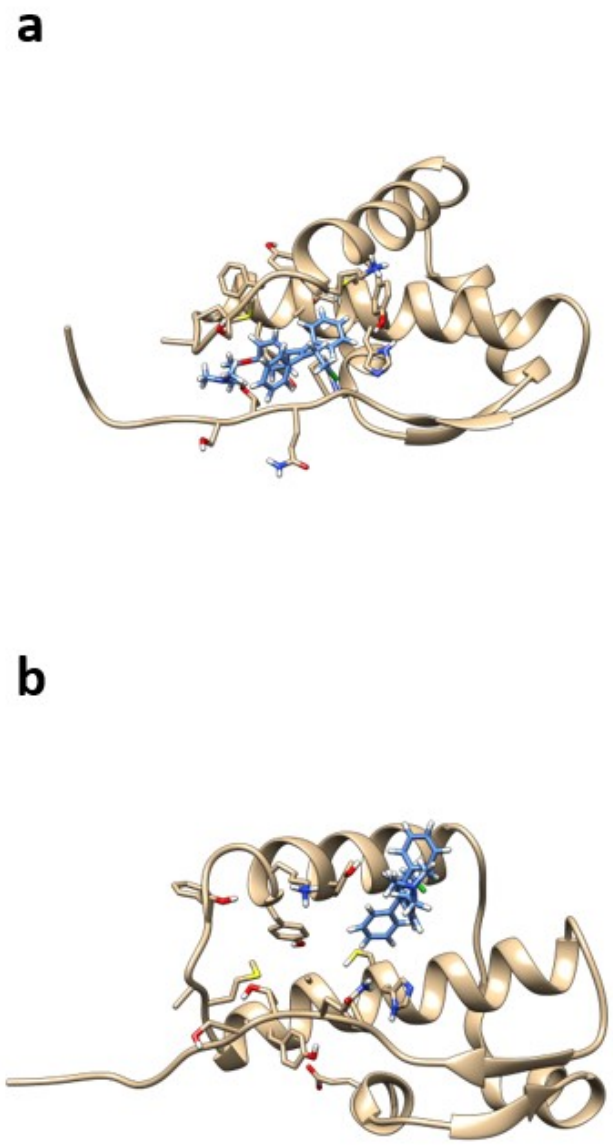

Figure S2: NSP4 in the initial docked conformation (a) and at 123.6 nanoseconds of simulation (b).

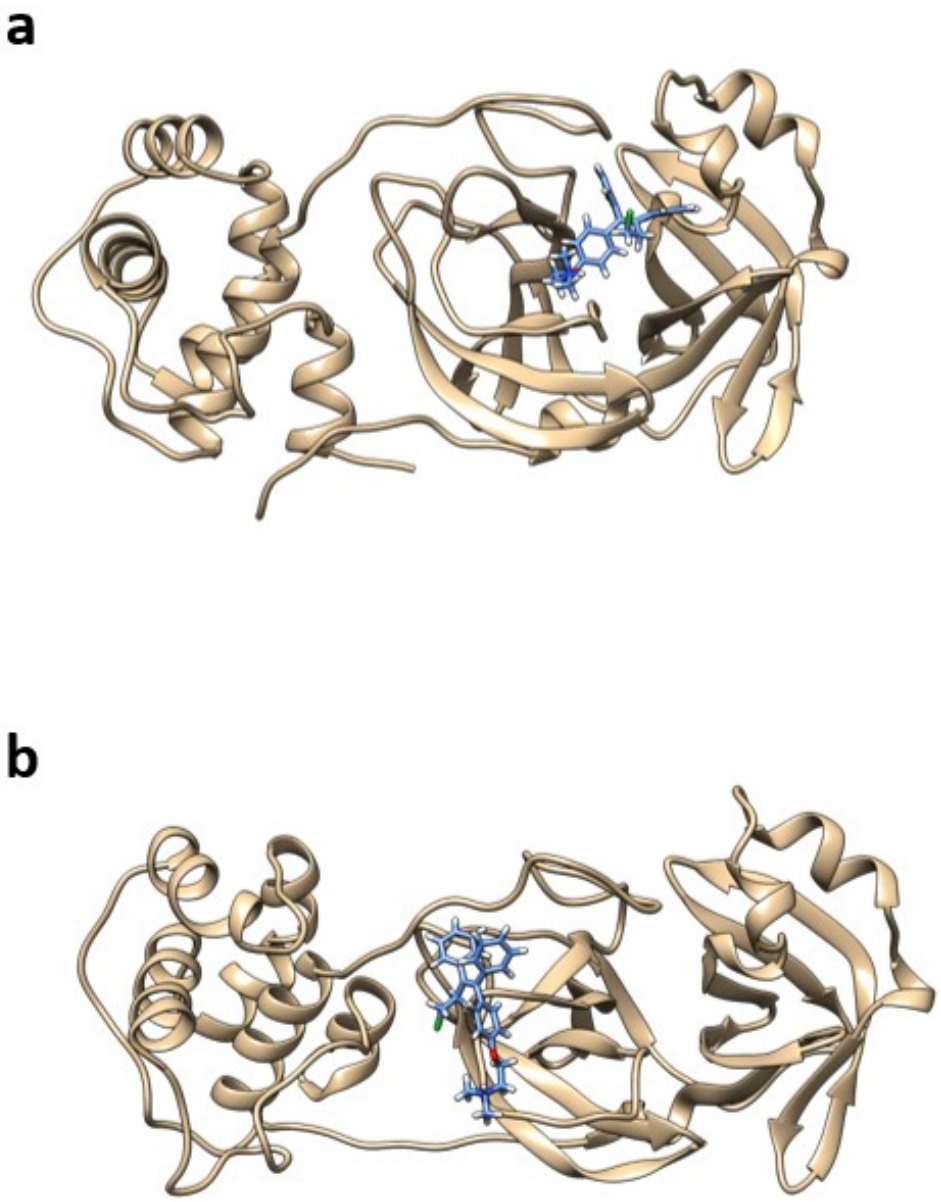

Figure S3: NSP5 (3CL-PRO) in its initial docked conformation (a) and at 284.2 nanoseconds of simulation (b).

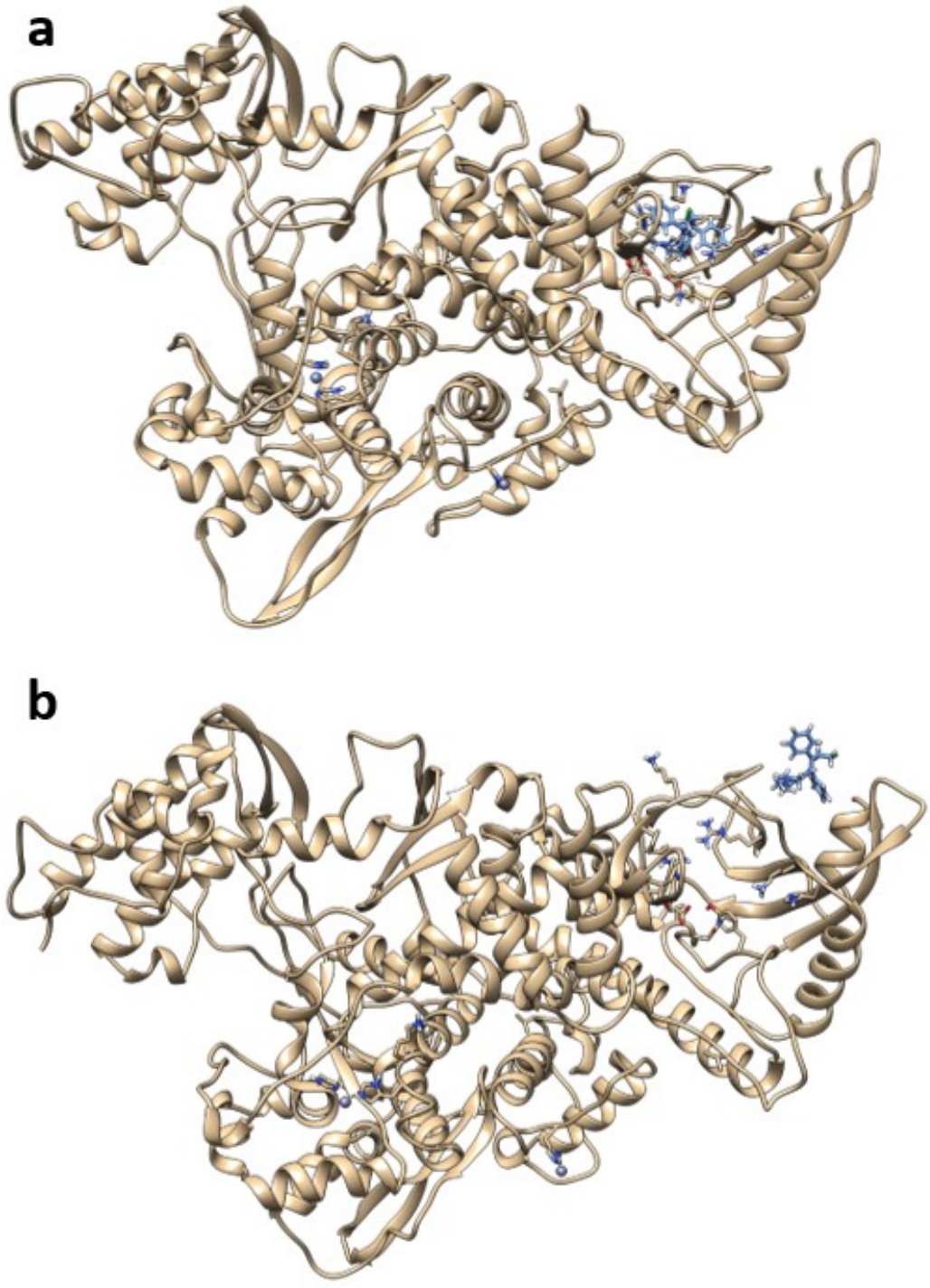

Figure S4: NSP12 (RNA-Polymerase) in its initial docked conformation (a) and at 60.4 nanoseconds of simulation (b).

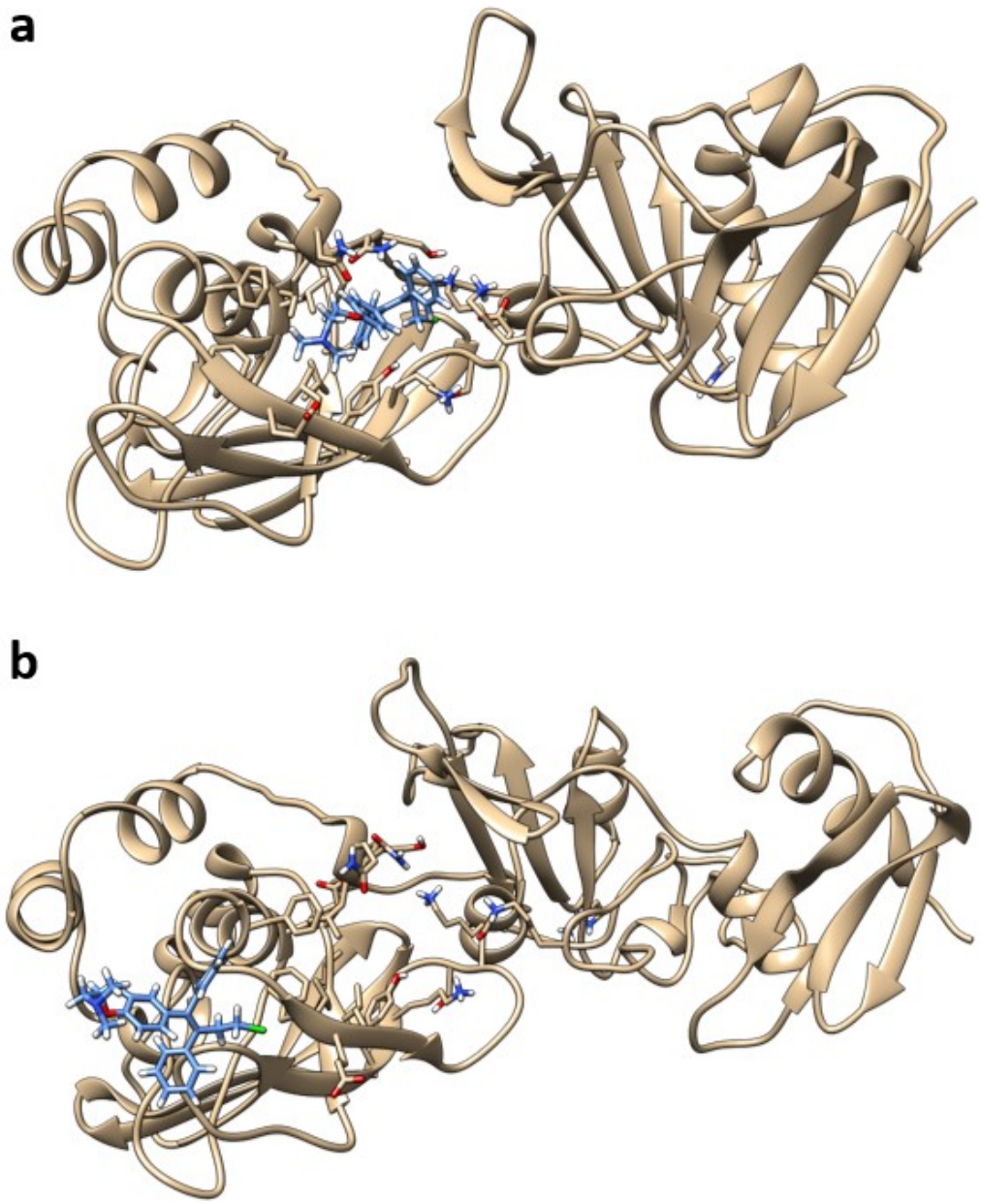

Figure S5: NSP15 in its initial docked conformation (a) and at 35.3 nanoseconds of simulation (b).

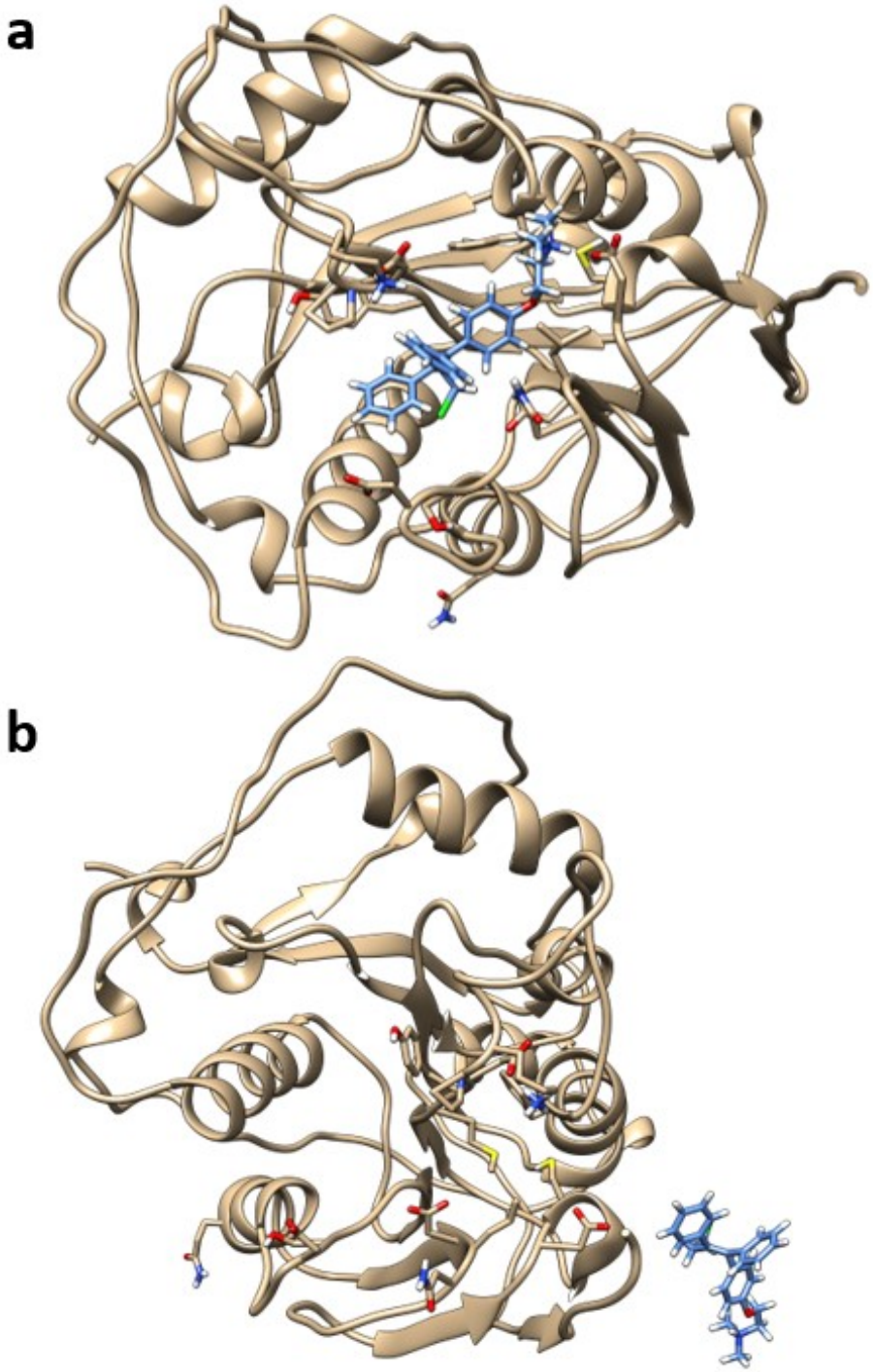

Figure S6: NSP16 in its initial docked conformation (a) and at 11.5 nanoseconds of simulation (b).

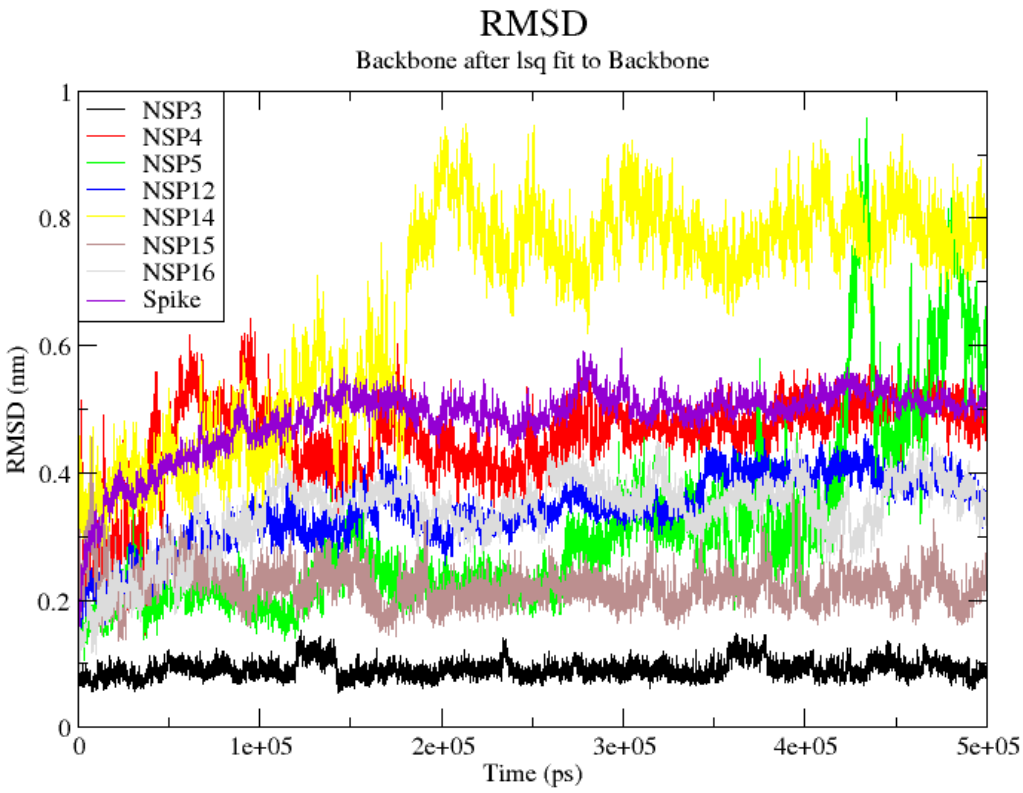

Figure S7: Root-Mean-Squared Deviation (RMSD) plot for all proteins simulated; each protein was submitted to 500 nanoseconds of molecular dynamics simulation.